A NEW ACTIVATED SLUDGE MODEL FOR INDUSTRIAL WASTEWATER TREATMENT FACILITIES

Oliver Schraa, Hugh Monteith, Spencer Snowling, and Hank Andres

Hydromantis, Inc.
1 James St. South, Suite 1601
Hamilton, Ontario, Canada L8P 4R5

ABSTRACT

A new activated sludge model, called MantisIW, has been developed for industrial wastewater treatment plants (WWTPs). The model provides a general modeling framework for industrial activated sludge plants and allows for flexibility in handling a wide variety of industrial wastewaters such as those encountered in the petroleum, petrochemical, organic chemical, pulp and paper, pharmaceutical, and food and beverage industries. MantisIW combines the ASM1 biological model (Henze *et al.*, 2000) with a revised categorization of the influent COD, multiple degradation and transformation pathways for the new COD categories, the modeling of sulfur compounds, colloidal material, and toxics, and the modeling of nutrient and alkalinity limitations on biological growth. The addition of partitioning to different media, including effluent, air emissions and residual solids captures the unique nature of the fate of industrial wastes. The default kinetic and stoichiometric parameter values in the model are taken from the literature and the TOXCHEM+ (Hydromantis, Inc., 2006b) predictive fate modeling package. Future work will include fine-tuning of the kinetic and stoichiometric parameter values using historical dynamic operating data from industrial WWTPs.

KEYWORDS

Modeling, simulation, activated sludge, industrial wastewater.

INTRODUCTION

Process modeling has become an accepted tool for the design and optimization of domestic wastewater treatment plants (WWTPs) (Henze *et al.*, 2000). This is in large part due to the development of standardized activated sludge models such as ASM1, ASM2d, and ASM3 (Henze *et al.*, 2000) and the increased availability of intuitive process simulation platforms. In contrast, activated sludge modeling is less common in the field of industrial wastewater treatment due to the unique nature of the wastewater and the extreme operating conditions often encountered. Existing activated sludge process (ASP) models can be used to model industrial WWTPs (e.g. Bury *et al.*, 2002; Goodfellow *et al.*, 2004; Schraa *et al.*, 2004; Stricker and Racault, 2005; Takács *et al.*, 1998), but model customization may be required to handle pollutants not commonly found in domestic wastewater. Direct application of the existing models is often possible in industries such as food processing (Snowling and Malyk, 2002), but

may be difficult in other industries, suggesting the need for a specialized industrial ASP model.

The objective of the current work is to develop a general modeling framework for industrial ASP's that allows for flexibility in handling a wide variety of industrial wastewaters such as those encountered in the petroleum, petrochemical, organic chemical, pulp and paper, pharmaceutical, and food and beverage industries.

MODEL DEVELOPMENT

Introduction

MantisIW is a dynamic-mechanistic model of the industrial activated sludge process. It is based on calculating dynamic mass balances for chemical oxygen demand (COD), nitrogen, phosphorus, and sulfur around completely-mixed or plug-flow activated sludge reactors. The general form of the mass balance equation is as follows:

Rate of	=	Rate of	-	Rate of	±	Rate of Production or Consumption by
Accumulation		Input		Output		Reaction or Physical Transformation

To calculate the production/consumption terms, the model utilizes aspects of the ASM1 (Henze *et al*., 2000), ASM2d (Henze *et al*., 2000), Mantis (Hydromantis, 2006a), and Baker (1994) biological models along with a revised categorization of the influent COD and added biological and physical transformations. The model has 32 components or state variables, for which mass balances are written, and 38 transformation processes that are incorporated into the production/consumption terms.

Model Components

In MantisIW, the model components or state variables are categorized as follows:

Existing ASM1 influent COD state variables

- Readily biodegradable substrate
- Slowly biodegradable substrate
- Soluble inert organic matter
- Particulate inert organic matter

New organic influent COD state variables

- Organic solvents
  - o Oxygenated
  - o Halogenated
- Aliphatic compounds
  - o Short-chain
  - o Long-chain

- Aromatic compounds
  - Mono-cyclic
  - Poly-cyclic
  - Halogenated
- Toxic or inhibitory compounds
- Colloidal material

The COD categorization was developed by considering the physical, chemical and biological properties (biodegradability, hydrophobicity and volatility of different organic compounds). Consideration was also given to the classes of compounds that are normally tracked in industrial WWTPs due to health, safety and environmental concerns. The new influent COD variables are further defined below and in Table 1, with accompanying typical and representative compounds in terms of biodegradability, hydrophobicity and volatility.

Dissolved Oxygen

Dissolved oxygen is required for aerobic biomass growth and prediction of aeration requirements.

Biomass Associated COD

COD variables are also included to represent biomass and include those in ASM1 plus an additional biomass type for sulfur oxidizing biomass:

- Active heterotrophic biomass
- Active autotrophic nitrifying biomass
- Active sulfur oxidizing biomass
- Particulate products resulting from biomass decay

Adsorbed COD

Certain types of difficult-to-degrade COD can be adsorbed onto the surface of the heterotrophic biomass in the model including:

- Adsorbed long-chain aliphatic compounds
- Adsorbed poly-cyclic aromatic compounds
- Adsorbed halogenated aromatic compounds
- Adsorbed colloidal material

Table 1 – Definition of New Influent COD Variables in MantisIW

New COD variable	Typical compounds	Representative compound
Oxygenated organic solvents	• Alcohols • Aldehydes and ketones • Carboxylic acids • Esters • Ethers	Methyl ethyl ketone
Halogenated organic solvents	• Alkyl halides • e.g. chloroform, carbon tetrachloride, methyl iodide	Chloroform
Short-chain aliphatic compounds	• Hydrocarbons with less than 18 carbon atoms including: alkanes, alkenes, alkynes, fats and oils	Methyl cyclohexane
Long-chain aliphatic compounds	• Hydrocarbons with 18 or more carbon atoms including: alkanes, alkenes, alkynes, fats and oils	Eicosane ($C_{20}H_{42}$)
Monocyclic aromatic compounds	• Aromatic compounds with single benzene ring • e.g. benzene, toluene, styrene, xylene	Ethyl benzene
Polycyclic aromatic compounds	• Aromatic compounds with multiple benzene rings • e.g. napthalene, phenanthrene, benzo[a]pyrene	Fluoranthene
Halogenated aromatic compounds	• Aryl halides • e.g. bromobenzene, chlorobenzene)	1,2,4-Trichlorobenzene
Toxic or inhibitory compounds	• Phenolic compounds	Phenol
Colloidal material	• Lignins	Lignins

Nitrogen Variables

The nitrogen variables include those in ASM1 and nitrogen gas:

- ammonia and ammonium nitrogen
- nitrate and nitrite nitrogen
- soluble organic nitrogen
- particulate organic nitrogen
- nitrogen gas

In addition, the biomass variables and the products from decay have associated nitrogen fractions.

Phosphorus Variables

Soluble phosphorus has been included as a state variable to account for possible phosphorus limitations which are common in industrial wastewater treatment. In addition, the biomass variables and the products from decay have associated phosphorus fractions.

Sulfur Variables

Following Baker (1994), the following sulfur variables have been included so that the impact of sulfur oxidation on aeration requirements can be modeled:

- Reduced sulfur compounds (e.g. sulfides, mercaptans)
- Sulfates

Inorganic Variables

Alkalinity is included to track potential changes in pH. Following the Mantis model (Hydromantis, 2006a), inert inorganic suspended solids are included so that the total suspended solids concentration can be calculated.

Table 2 presents a summary of the model components or state variables including symbols and units. Mass balances are written for all of these components in the model.

Table 2 – Definition of Component Nomenclature in MantisIW Model

Symbol	Soluble/Particulate	Definition	Units
S_S	soluble	Readily biodegradable substrate	mg COD/L
X_S	particulate	Slowly biodegradable substrate	mg COD/L
S_I	soluble	Soluble inert organic matter	mg COD/L
X_I	particulate	Particulate inert organic matter	mg COD/L
X_U	particulate	Particulate products arising from biomass decay	mg COD/L
S_{OS}	soluble	Oxygenated organic solvents	mg COD/L
S_{HS}	soluble	Halogenated organic solvents	mg COD/L
S_{ALSC}	soluble	Short-chain aliphatic compounds	mg COD/L
S_{ALLC}	soluble	Long-chain aliphatic compounds	mg COD/L
X_{ALLC}	particulate	Adsorbed long-chain aliphatic compounds	mg COD/L
S_{ARM}	soluble	Mono-cyclic aromatic compounds	mg COD/L
S_{ARP}	soluble	Poly-cyclic aromatic compounds	mg COD/L
X_{ARP}	particulate	Adsorbed poly-cyclic aromatic compounds	mg COD/L
S_{ARH}	soluble	Halogenated aromatic compounds	mg COD/L
X_{ARH}	particulate	Adsorbed halogenated aromatic compounds	mg COD/L
S_{PH}	soluble	Toxic or inhibitory compounds	mg COD/L
S_{COL}	soluble	Colloidal material	mg COD/L
X_{COL}	particulate	Adsorbed colloidal material	mg COD/L
S_O	soluble	Dissolved oxygen	mg -COD/L
X_{BH}	particulate	Active heterotrophic biomass	mg COD/L
X_{BA}	particulate	Active autotrophic nitrifying biomass	mg COD/L
X_{BS}	particulate	Active sulfur oxidizing biomass	mg COD/L
S_{NH}	soluble	Ammonia or ammonium nitrogen	mg N/L
S_{NO}	soluble	Nitrate and nitrite nitrogen	mg N/L
S_{ND}	soluble	Soluble organic nitrogen	mg N/L
X_{ND}	particulate	Particulate organic nitrogen	mg N/L
S_{NN}	soluble	Dinitrogen	mg N/L
S_P	soluble	Soluble ortho-phosphate	mg P/L
S_{SO}	soluble	Sulfate sulfur	mg S/L
S_{SR}	soluble	Reduced sulfur	mg S/L
S_{ALK}	soluble	Alkalinity	mole HCO_3^- /m^3
X_{II}	particulate	Inert inorganic suspended solids	mg/L

Model Processes

The MantisIW model includes the following transformation processes:

- *Aerobic and anoxic growth of heterotrophs on biodegradable substrate*
- *Inhibited aerobic and anoxic growth of heterotrophs on toxic compounds*
- *Adsorption and subsequent aerobic/anoxic heterotrophic growth on adsorbed substrate*
- *Volatilization due to surface evaporation and air stripping*
- *Hydrolysis of slowly biodegradable substrate and particulate organic nitrogen*
- *Decay of heterotrophs*
- *Ammonification of soluble organic nitrogen to ammonia*
- *Aerobic growth and decay of nitrifiers*
- *Aerobic growth and decay of sulfur oxidizing organisms*

The influent COD components can undergo one or more transformation processes depending on their individual characteristics. The possible transformations for each influent COD component in the model are described in Table 3.

Table 3 – Possible Transformations for Influent COD Components in MantisIW Model

Type of Organic Compound	COD Components Included	Possible Transformations
Readily biodegradable, soluble, non-volatile	• Readily biodegradable substrate	• Aerobic/anoxic heterotrophic growth
Slowly biodegradable, particulate	• Slowly biodegradable substrate	• Hydrolysis to readily biodegradable substrate
Readily biodegradable, soluble, volatile	• Oxygenated solvents • Halogenated solvents • Short-chain aliphatic compounds • Mono-cyclic aromatic compounds	• Aerobic/anoxic heterotrophic growth • Volatilization
Biodegradable toxic or inhibitory compounds	• Phenol	• Inhibited aerobic/anoxic heterotrophic growth • Volatilization
Partially miscible, non-volatile	• Long-chain aliphatic compounds • Poly-cyclic aromatic compounds • Colloidal material	• Adsorption • Aerobic/anoxic heterotrophic growth on adsorbed material
Partially miscible, volatile	• Halogenated aromatic compounds	• Adsorption • Aerobic/anoxic heterotrophic growth on adsorbed material • Volatilization

The following features are incorporated into the MantisIW model:

- Simultaneous nitrification/denitrification (if applicable)
- Ammonium uptake as part of biological growth
- Phosphorus uptake as part of biological growth
- Alkalinity impact on biological growth

The COD transformation processes in MantisIW are presented in Figure 1 (overview of COD transformations) and Figure 2 (overview of biological growth processes). The transformations are shown along with the required electron acceptors and nutrients.

Figure 1 – Overview of COD Transformation Processes in MantisIW (Adsorption, Volatilization, and Heterotrophic Growth/Decay)
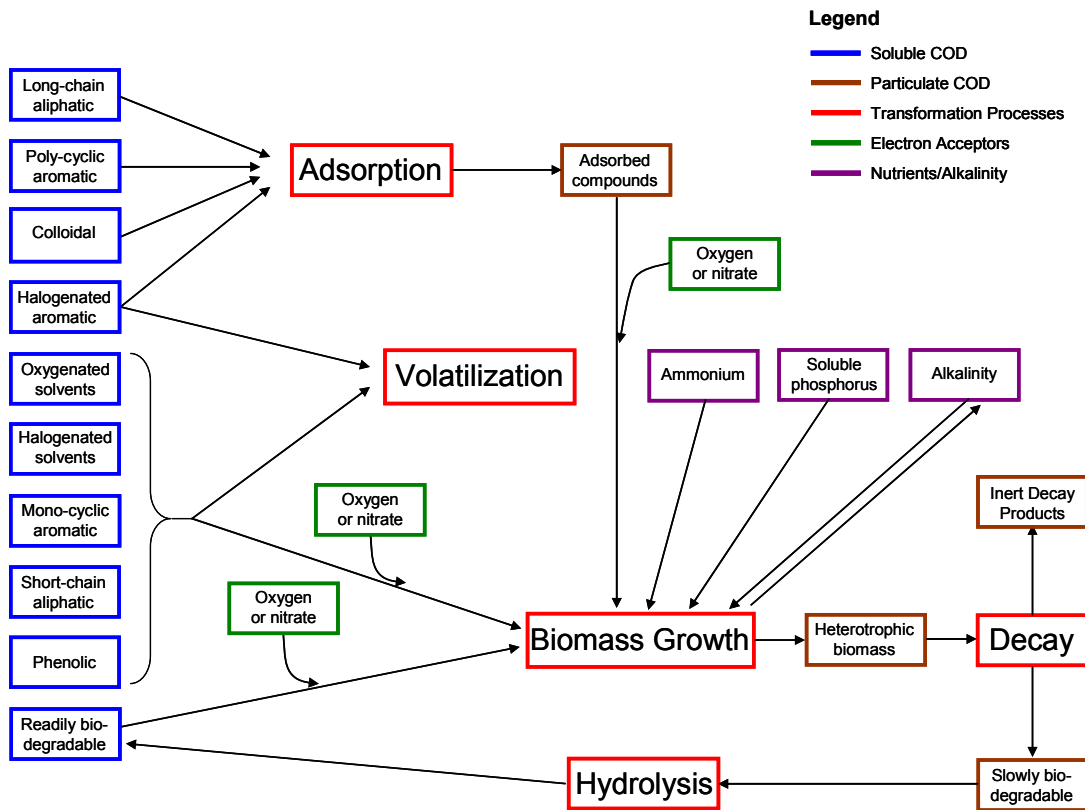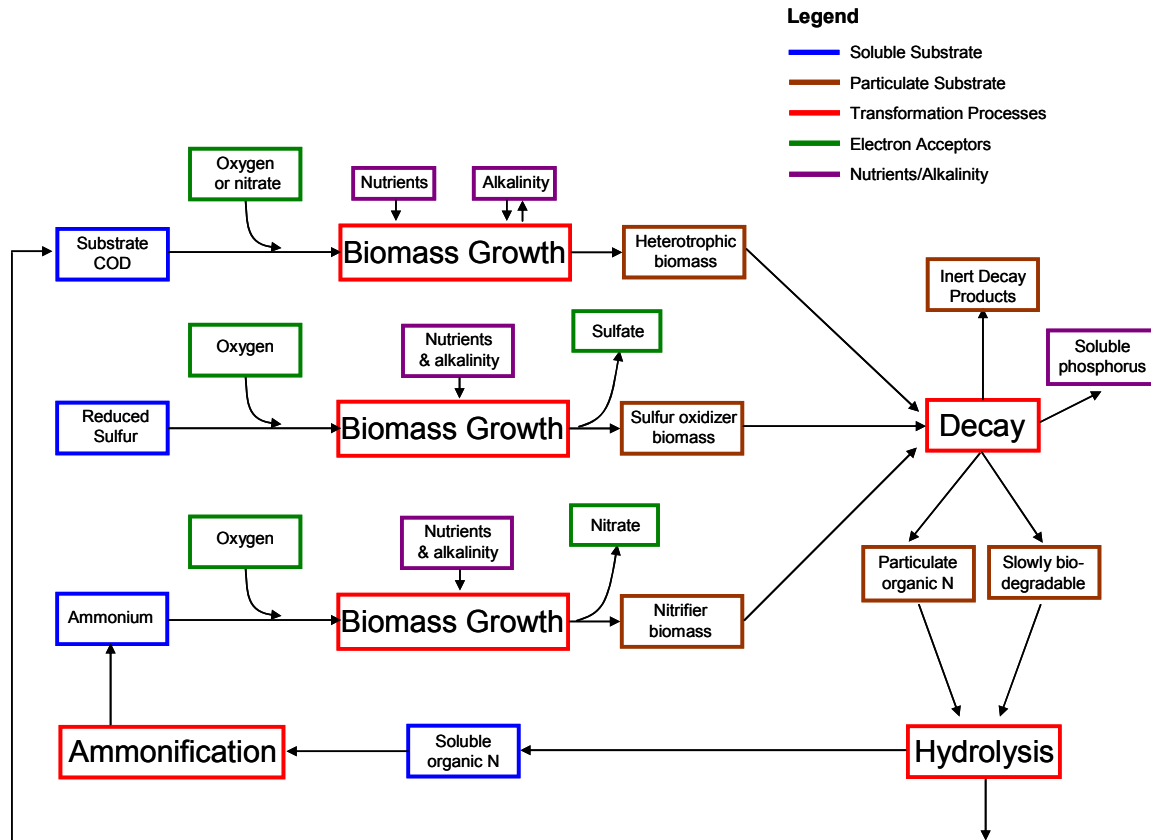
Figure 2 – Overview of Biological Growth Processes in MantisIW

The model processes and process rate equations are described below. Processes and rate equations that are identical to those in ASM1 are not described.

Aerobic and Anoxic Growth of Heterotrophs on Biodegradable Substrate

In MantisIW, heterotrophs can grow under aerobic and anoxic conditions on the following soluble substrates: readily biodegradable substrate (as in ASM1), oxygenated solvents, halogenated solvents, short-chain aliphatic compounds, and mono-cyclic aromatic compounds. Switching functions have been added, as in ASM2d, to limit biomass growth if ammonium, ortho-phosphate, or alkalinity concentrations are low.

The general rate expression used for aerobic growth of heterotrophs is given below:

$$\rho_{Het,\,Aer,\,S_j} = \mu_{H,\,j} \times \left(\frac{S_j}{K_{S,\,j} + S_j} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$$

where:

$S_j \equiv S_S$, S_{OS}, S_{HS}, S_{ALSC}, or S_{ARM}

$\rho_{Het,Aer,S_j} \equiv$ rate of aerobic growth of heterotrophs on the substrate S_j (mg COD/L·d)

$\mu_{H,j} \equiv$ maximum specific growth rate on S_j (1/d)

$K_{S,j} \equiv$ half-saturation coefficient for S_j (mg COD/L)

Similarly, the general rate expression used for anoxic growth of heterotrophs is as follows:

$$\rho_{Het,Anox,S_j} = \eta_g \times \mu_{H,j} \times \left(\frac{S_j}{K_{S,j} + S_j} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$$

where:

$\rho_{Het,Anox,S_j} \equiv$ rate of anoxic growth of heterotrophs on substrate S_j (mg COD/L·d)

$\eta_g \equiv$ anoxic reduction factor for maximum specific growth rate

The switching function *AirNo* can be replaced with *AllowNitDenit* in the above equation if simultaneous nitrification/denitrification is being modeled. The K_{AD} parameter (see Table 7) allows independent adjustment of denitrification without affecting the aerobic processes that use K_{OH}.

Inhibited Aerobic and Anoxic Growth of Heterotrophs on Toxic Compounds

Certain compounds such as phenols can be inhibitory to biomass growth with the inhibition effect increasing at higher phenol concentrations. The Haldane equation (Gaudy and Gaudy, 1980) is used to model inhibition as done by Baker (1994) in the following rate equation:

$$\rho_{Het,Aer,S_{PH}} = \mu_{H,PH} \times \left(\frac{S_{PH}}{K_{S,PH} + S_{PH} + \frac{S_{PH}^2}{K_{I,PH}}} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$$

An alkalinity switching function has been added to the above equation, in MantisIW, to limit growth at low alkalinity concentrations.

Similarly, the following rate expression is used for inhibited anoxic growth of heterotrophs:

$$\rho_{Het,Anox,S_{PH}} = \eta_g \times \mu_{H,PH} \times \left(\frac{S_{PH}}{K_{S,PH} + S_{PH} + \frac{S_{PH}^2}{K_{I,PH}}} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$$

Adsorption and Subsequent Aerobic/Anoxic Heterotrophic Growth on Adsorbed Substrate

Compounds such as long-chain hydrocarbons are large molecules that are only partially miscible in water and are more difficult to degrade than compounds such as oxygenated solvents. Following Baker (1994), it is postulated that these molecules are first adsorbed onto the surface of the biomass, and then hydrolyzed and biologically degraded. The rate of adsorption, modified in MantisIW to allow for multiple types of adsorbed substrate, is defined as follows:

$$\rho_{Ads, S_l} = K_{A,l} \times \max\left(\left(F_{\max} - \frac{X_{ALLC} + X_{ARP} + X_{ARH} + X_{COL}}{X_{BH}}\right), 0\right) \times S_l \times X_{BH}$$

where:

$S_l \equiv S_{ALLC}, S_{ARP}, S_{ARH},$ or S_{COL}

$F_{\max} \equiv$ Maximum number of sites for adsorption

$K_{A,l} \equiv$ Adsorption rate for S_l

Following adsorption, aerobic growth of heterotrophs occurs using the adsorbed long-chain aliphatic compounds, poly-cyclic aromatic compounds, halogenated aromatic compounds, and colloidal material as substrate. In this case, the Monod expression for the substrate is written in terms of the surface concentration of the adsorbed substrate on the heterotrophic biomass which is estimated by the ratio X_l/X_{BH}. The general rate expression used is given below:

$$\rho_{Het, Aer, X_l} = \mu_{H,l} \times \left(\frac{\frac{X_l}{X_{BH}}}{K_{S,l} + \frac{X_l}{X_{BH}}}\right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$$

where:

$X_l \equiv X_{ALLC}, X_{ARP}, X_{ARH},$ or X_{COL}

$\rho_{Het, Aer, X_l} \equiv$ rate of aerobic growth of heterotrophs on adsorbed substrate X_l (mg COD/L·d)

As with growth on soluble substrates, biomass growth is limited at low ammonium, ortho-phosphate, and alkalinity concentrations. The alkalinity switching function is not used in the Baker (1994) model.

Anoxic growth of heterotrophs is also defined on the adsorbed long-chain aliphatic compounds, poly-cyclic aromatic compounds, halogenated aromatic compounds, and colloidal material. The rate expression used is given below:

$$\rho_{Het,\,Anox,\,X_l} = \eta_g \times \mu_{H,\,l} \times \left(\frac{\dfrac{X_l}{X_{BH}}}{K_{S,\,l} + \dfrac{X_l}{X_{BH}}} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$$

where:

$\rho_{Het,\,Anox,\,X_l} \equiv$ rate of anoxic growth of heterotrophs on adsorbed substrate X_l (mg COD/L·d)

Volatilization Due to Surface Evaporation and Air Stripping

Many organic compounds are volatile and subject to surface evaporation and air stripping due to diffused aeration systems. In MantisIW, the rate of volatilization for oxygenated solvents, halogenated solvents, short-chain aliphatic compounds, mono-cyclic aromatic compounds, phenols (toxic compounds), and halogenated aromatic compounds is calculated as the sum of surface volatilization losses and the air stripping losses as shown below:

$$\rho_{Vol,\,S_j} = \left(k_{V,\,j} + k_{STRIP,\,j} \right) \times S_j$$

where:

$S_j \equiv S_{OS}, S_{HS}, S_{ALSC}, S_{ARM}, S_{PH},$ or S_{ARH}
$k_{V,\,j} \equiv$ surface evaporation rate (1/d)
$k_{STRIP,\,j} \equiv$ air stripping rate (1/d)

The air stripping rate is defined as

$$k_{STRIP,\,j} = \frac{Q_{air} \times f_j \times H_j}{V}$$

with:

$Q_{air} \equiv$ diffused air flow to activated sludge reactor at field conditions, m^3/d
$f_j \equiv$ fractional saturation of gas bubbles with S_j, dimensionless
$H_j \equiv$ Henry's law coefficient for S_j, m^3 liquid/m^3 gas
$V \equiv$ volume of activated sludge reactor

The fractional saturation is defined using the following equation proposed by Matter-Muller *et al.* (1981):

$$f_j = 1 - \exp\left(\frac{-K_L a \times V}{Q_{air} \times H_j} \right)$$

with $K_La \equiv$ oxygen mass transfer coefficient (1/d).

Aerobic Growth and Decay of Nitrifiers

These processes are modeled as in ASM1 except that phosphorus and alkalinity switching functions have been added to the aerobic growth rate equation.

Aerobic Growth and Decay of Sulfur Oxidizing Organisms

Reduced sulfur compounds can be found in high concentrations in petroleum, petrochemical, and pulp and paper wastewater. Sulfur oxidizing organisms are capable of oxidizing the reduced sulfur to sulfate, which can lead to a significant oxygen demand. The following equation is used to model the rate of sulfur oxidation (growth of sulfur oxidizers) as in Baker (1994) but with added alkalinity and phosphorus switching functions:

$$\rho_{Sulfur,Growth} = \mu_{A,Sulfur} \times \left(\frac{S_{SR}}{K_{S,Sulfur} + S_{SR}} \right) \times X_{BS} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$$

The effect of sulfur oxidation on alkalinity has also been added to the model in MantisIW. Sulfur oxidizer decay is modeled as follows:

$$\rho_{Sulfur,Decay} = b_{A,Sulfur} \times X_{BS}$$

Model Stoichiometry and Kinetics

The MantisIW reaction stoichiometry is shown in Table 4. See Henze *et al*. (2000) for a description of the matrix approach to presenting biokinetic reaction stoichiometry. The process rate equations and switching functions are shown in Table 5 and Table 7, respectively.

The model parameters are defined in Table 6 and Tables 8 through 12. The parameter values are taken from the literature and other sources. The parameters for existing ASM1 processes are taken from the Mantis model (Hydromantis, 2006a), found in GPS-X™. This parameter set has been found to be applicable to a variety of wastewaters, including domestic and readily biodegradable industrial wastewaters. These parameters are also applied in MantisIW to biological growth on oxygenated and halogenated solvents, and mono-cyclic aromatic compounds, as these are considered readily biodegradable. For biological growth on short-chain aliphatic compounds, phenols, adsorbed long-chain aliphatic compounds, and reduced sulfur compounds, the kinetics and stoichiometry are taken from Baker (1994). The impact of sulfur oxidation on alkalinity was derived as part of the current work. The parameter values for the adsorption and volatilization processes and biological growth on the remaining adsorbed compounds are taken from the TOXCHEM+™ (Hydromantis, 2006b) predictive fate modeling package. The kinetic rate parameters in MantisIW are temperature dependent, with temperature dependency modeled using the Arrhenius temperature correlation. The actual parameter values used are not presented due to space limitations and will be provided in a future publication.

Table 4 – MantisIW Stoichiometric Matrix (Part 1)

Process	S_S	S_j	S_l	S_{ARH}	S_{PH}	S_O
Aerobic growth of heterotrophs on S_S	$\dfrac{-1}{Y_H}$					$\dfrac{-(1-Y_H)}{Y_H}$
Anoxic growth of heterotrophs on S_S	$\dfrac{-1}{Y_H}$					
Aerobic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})		$\dfrac{-1}{Y_{H,j}}$				$\dfrac{-(1-Y_{H,j})}{Y_{H,j}}$
Anoxic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})		$\dfrac{-1}{Y_{H,j}}$				
Aerobic growth of heterotrophs on S_{PH}					$\dfrac{-1}{Y_{H,PH}}$	$\dfrac{-(1-Y_{H,PH})}{Y_{H,PH}}$
Anoxic growth of heterotrophs on S_{PH}					$\dfrac{-1}{Y_{H,PH}}$	
Adsorption of S_l ($S_l = S_{ALLC}$, S_{ARP}, or S_{COL})			-1			
Adsorption of S_{ARH}				-1		
Aerobic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})						$\dfrac{-(1-Y_{H,l})}{Y_{H,l}}$
Anoxic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})						
Aerobic growth of heterotrophs on adsorbed X_{ARH}						$\dfrac{-(1-Y_{H,ARH})}{Y_{H,ARH}}$
Anoxic growth of heterotrophs on adsorbed X_{ARH}						
Volatilization of S_j		-1				
Volatilization of S_{ARH}				-1		
Volatilization of S_{PH}					-1	
Decay of heterotrophs						
Aerobic growth of sulfur oxidizers						$\dfrac{-(2-Y_{Sulfur})}{Y_{Sulfur}}$
Decay of sulfur oxidizers						
Aerobic growth of nitrifiers						$\dfrac{-(4.57-Y_A)}{Y_A}$
Decay of nitrifiers						
Hydrolysis of entrapped organics	1					
Hydrolysis of entrapped organic nitrogen						
Ammonification of soluble organic nitrogen						

Table 4 – MantisIW Stoichiometric Matrix (Part 2)

Process	S_I	X_S	X_{BH}	X_{BA}	X_{BS}	X_l	X_{ARH}	X_I
Aerobic growth of heterotrophs on S_S			1					
Anoxic growth of heterotrophs on S_S			1					
Aerobic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})			1					
Anoxic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})			1					
Aerobic growth of heterotrophs on S_{PH}			1					
Anoxic growth of heterotrophs on S_{PH}			1					
Adsorption of S_l ($S_l = S_{ALLC}$, S_{ARP}, or S_{COL})						1		
Adsorption of S_{ARH}							1	
Aerobic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})			1			$\dfrac{-1}{Y_{H,l}}$		
Anoxic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})			1			$\dfrac{-1}{Y_{H,l}}$		
Aerobic growth of heterotrophs on adsorbed X_{ARH}			1				$\dfrac{-1}{Y_{H,ARH}}$	
Anoxic growth of heterotrophs on adsorbed X_{ARH}			1				$\dfrac{-1}{Y_{H,ARH}}$	
Volatilization of S_j								
Volatilization of S_{ARH}								
Volatilization of S_{PH}								
Decay of heterotrophs		1-f_u	-1					
Aerobic growth of sulfur oxidizers					1			
Decay of sulfur oxidizers		1-f_u			-1			
Aerobic growth of nitrifiers				1				
Decay of nitrifiers		1-f_u		-1				
Hydrolysis of entrapped organics		-1						
Hydrolysis of entrapped organic nitrogen								
Ammonification of soluble organic nitrogen								

Table 4 – MantisIW Stoichiometric Matrix (Part 3)

Process	X_U	X_{II}	S_{NH}	S_{NO}	S_{NN}	S_{ND}
Aerobic growth of heterotrophs on S_S			$-ixbn$			
Anoxic growth of heterotrophs on S_S			$-ixbn$	$\dfrac{-(1-Y_H)}{2.86 \times Y_H}$	$\dfrac{(1-Y_H)}{2.86 \times Y_H}$	
Aerobic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})			$-ixbn$			
Anoxic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})			$-ixbn$	$\dfrac{-(1-Y_{H,j})}{2.86 \times Y_{H,j}}$	$\dfrac{(1-Y_{H,j})}{2.86 \times Y_{H,j}}$	
Aerobic growth of heterotrophs on S_{PH}			$-ixbn$			
Anoxic growth of heterotrophs on S_{PH}			$-ixbn$	$\dfrac{-(1-Y_{H,PH})}{2.86 \times Y_{H,PH}}$	$\dfrac{(1-Y_{H,PH})}{2.86 \times Y_{H,PH}}$	
Adsorption of S_l ($S_l = S_{ALLC}$, S_{ARP}, or S_{COL})						
Adsorption of S_{ARH}						
Aerobic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})			$-ixbn$			
Anoxic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})			$-ixbn$	$\dfrac{-(1-Y_{H,l})}{2.86 \times Y_{H,l}}$	$\dfrac{(1-Y_{H,l})}{2.86 \times Y_{H,l}}$	
Aerobic growth of heterotrophs on adsorbed X_{ARH}			$-ixbn$			
Anoxic growth of heterotrophs on adsorbed X_{ARH}			$-ixbn$	$\dfrac{-(1-Y_{H,ARH})}{2.86 \times Y_{H,ARH}}$	$\dfrac{(1-Y_{H,ARH})}{2.86 \times Y_{H,ARH}}$	
Volatilization of S_j						
Volatilization of S_{ARH}						
Volatilization of S_{PH}						
Decay of heterotrophs						
Aerobic growth of sulfur oxidizers			$-ixbn$			
Decay of sulfur oxidizers						
Aerobic growth of nitrifiers			$-ixbn - \dfrac{1}{Y_A}$	$\dfrac{1}{Y_A}$		
Decay of nitrifiers						
Hydrolysis of entrapped organics						
Hydrolysis of entrapped organic nitrogen						1
Ammonification of soluble organic nitrogen			1			-1

Table 4 – MantisIW Stoichiometric Matrix (Part 4)

Process	X_{ND}	S_P	S_{SR}	S_{SO}
Aerobic growth of heterotrophs on S_S		-*ixbp*		
Anoxic growth of heterotrophs on S_S		-*ixbp*		
Aerobic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})		-*ixbp*		
Anoxic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})		-*ixbp*		
Aerobic growth of heterotrophs on S_{PH}		-*ixbp*		
Anoxic growth of heterotrophs on S_{PH}		-*ixbp*		
Adsorption of S_l ($S_l = S_{ALLC}$, S_{ARP}, or S_{COL})				
Adsorption of S_{ARH}				
Aerobic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})		-*ixbp*		
Anoxic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})		-*ixbp*		
Aerobic growth of heterotrophs on adsorbed X_{ARH}		-*ixbp*		
Anoxic growth of heterotrophs on adsorbed X_{ARH}		-*ixbp*		
Volatilization of S_j				
Volatilization of S_{ARH}				
Volatilization of S_{PH}				
Decay of heterotrophs	*ixbn* - $f_u \times$ *iuxn*	*ixbp* - $f_u \times$ *iuxp*		
Aerobic growth of sulfur oxidizers		-*ixbp*	$\dfrac{-1}{Y_{Sulfur}}$	$\dfrac{1}{Y_{Sulfur}}$
Decay of sulfur oxidizers	*ixbn* - $f_u \times$ *iuxn*	*ixbsp* - $f_u \times$ *iuxp*		
Aerobic growth of nitrifiers				
Decay of nitrifiers	*ixbn* - $f_u \times$ *iuxn*	*ixbp* - $f_u \times$ *iuxp*		
Hydrolysis of entrapped organics				
Hydrolysis of entrapped organic nitrogen	-1			
Ammonification of soluble organic nitrogen				

Table 4 – MantisIW Stoichiometric Matrix (Part 5)

Process	S_{ALK}
Aerobic growth of heterotrophs on S_S	$-ixbn/14$
Anoxic growth of heterotrophs on S_S	$\dfrac{(1-Y_H)}{14 \times 2.86 \times Y_H} - \dfrac{ixbn}{14}$
Aerobic growth of heterotrophs on S_j $(S_j = S_{OS}, S_{HS}, S_{ALSC},$ or $S_{ARM})$	$-ixbn/14$
Anoxic growth of heterotrophs on S_j $(S_j = S_{OS}, S_{HS}, S_{ALSC},$ or $S_{ARM})$	$\dfrac{(1-Y_{H,j})}{14 \times 2.86 \times Y_{H,j}} - \dfrac{ixbn}{14}$
Aerobic growth of heterotrophs on S_{PH}	$-ixbn/14$
Anoxic growth of heterotrophs on S_{PH}	$\dfrac{(1-Y_{H,PH})}{14 \times 2.86 \times Y_{H,PH}} - \dfrac{ixbn}{14}$
Adsorption of S_l $(S_l = S_{ALLC}, S_{ARP},$ or $S_{COL})$	
Adsorption of S_{ARH}	
Aerobic growth of heterotrophs on adsorbed X_l $(X_l = X_{ALLC}, X_{ARP},$ or $X_{COL})$	$-ixbn/14$
Anoxic growth of heterotrophs on adsorbed X_l $(X_l = X_{ALLC}, X_{ARP},$ or $X_{COL})$	$\dfrac{(1-Y_{H,l})}{14 \times 2.86 \times Y_{H,l}} - \dfrac{ixbn}{14}$
Aerobic growth of heterotrophs on adsorbed X_{ARH}	$-ixbn/14$
Anoxic growth of heterotrophs on adsorbed X_{ARH}	$\dfrac{(1-Y_{H,ARH})}{14 \times 2.86 \times Y_{H,ARH}} - \dfrac{ixbn}{14}$
Volatilization of S_j	
Volatilization of S_{ARH}	
Volatilization of S_{PH}	
Decay of heterotrophs	
Aerobic growth of sulfur oxidizers	$-\dfrac{ixbn}{14} - \dfrac{1}{3 \times Y_{Sulfur}}$
Decay of sulfur oxidizers	
Aerobic growth of nitrifiers	$-\dfrac{ixbn}{14} - \dfrac{1}{7 \times Y_A}$
Decay of nitrifiers	
Hydrolysis of entrapped organics	
Hydrolysis of entrapped organic nitrogen	
Ammonification of soluble organic nitrogen	$\dfrac{1}{14}$

Table 5 – MantisIW Process Rates (Part 1)

Process	Process Rate (mg COD/L·d or mg N/L·d)
Aerobic growth of heterotrophs on S_S	$\mu_H \times \left(\dfrac{S_S}{K_S + S_S} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Anoxic growth of heterotrophs on S_S	$\eta_g \times \mu_H \times \left(\dfrac{S_S}{K_S + S_S} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$
Aerobic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})	$\mu_{H,j} \times \left(\dfrac{S_j}{K_{S,j} + S_j} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Anoxic growth of heterotrophs on S_j ($S_j = S_{OS}$, S_{HS}, S_{ALSC}, or S_{ARM})	$\eta_g \times \mu_{H,j} \times \left(\dfrac{S_j}{K_{S,j} + S_j} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$
Aerobic growth of heterotrophs on S_{PH}	$\mu_{H,PH} \times \left(\dfrac{S_{PH}}{K_{S,PH} + S_{PH} + \dfrac{S_{PH}^2}{K_{I,PH}}} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Anoxic growth of heterotrophs on S_{PH}	$\eta_g \times \mu_{H,PH} \times \left(\dfrac{S_{PH}}{K_{S,PH} + S_{PH} + \dfrac{S_{PH}^2}{K_{I,PH}}} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$
Adsorption of S_l ($S_l = S_{ALLC}$, S_{ARP}, or S_{COL})	$K_{A,l} \times \max\left(\left(F_{max} - \dfrac{X_{ALLC} + X_{ARP} + X_{ARH} + X_{COL}}{X_{BH}} \right), 0 \right) \times S_l \times X_{BH}$
Adsorption of S_{ARH}	$K_{A,ARH} \times \max\left(\left(F_{max} - \dfrac{X_{ALLC} + X_{ARP} + X_{ARH} + X_{COL}}{X_{BH}} \right), 0 \right) \times S_{ARH} \times X_{BH}$
Aerobic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})	$\mu_{H,l} \times \left(\dfrac{\dfrac{X_l}{X_{BH}}}{K_{S,l} + \dfrac{X_l}{X_{BH}}} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Anoxic growth of heterotrophs on adsorbed X_l ($X_l = X_{ALLC}$, X_{ARP}, or X_{COL})	$\eta_g \times \mu_{H,l} \times \left(\dfrac{\dfrac{X_l}{X_{BH}}}{K_{S,l} + \dfrac{X_l}{X_{BH}}} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$
Aerobic growth of heterotrophs on adsorbed X_{ARH}	$\mu_{H,ARH} \times \left(\dfrac{\dfrac{X_{ARH}}{X_{BH}}}{K_{S,ARH} + \dfrac{X_{ARH}}{X_{BH}}} \right) \times X_{BH} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Anoxic growth of heterotrophs on adsorbed X_{ARH}	$\eta_g \times \mu_{H,ARH} \times \left(\dfrac{\dfrac{X_{ARH}}{X_{BH}}}{K_{S,l} + \dfrac{X_{ARH}}{X_{BH}}} \right) \times X_{BH} \times AirNo \times NO_3Yes \times NH_3Yes \times PO_4Yes \times AlkYes$
Volatilization of S_j	$\left(k_{V,j} + k_{STRIP,j} \right) \times S_j$
Volatilization of S_{ARH}	$\left(k_{V,ARH} + k_{STRIP,ARH} \right) \times S_{ARH}$
Volatilization of S_{PH}	$\left(k_{V,PH} + k_{STRIP,PH} \right) \times S_{PH}$
Decay of heterotrophs	$b_H \times X_{BH}$

Table 5 – MantisIW Process Rates (Part 2)

Process	Process Rate (mg COD/L·d or mg N/L·d)
Aerobic growth of sulfur oxidizers	$\mu_{A,Sulfur} \times \left(\dfrac{S_{SR}}{K_{S,Sulfur} + S_{SR}} \right) \times X_{BS} \times HetAirYes \times NH_3Yes \times PO_4Yes \times AlkYes$
Decay of sulfur oxidizers	$b_{A,Sulfur} \times X_{BS}$
Aerobic growth of nitrifiers	$\mu_A \times \left(\dfrac{S_{NH}}{K_{NA} + S_{NH}} \right) \times X_{BA} \times NitAirYes \times PO_4Yes \times AlkYes$
Decay of nitrifiers	$b_A \times X_{BA}$
Hydrolysis of entrapped organics	$k_H \times \left(\dfrac{\dfrac{X_S}{X_{BH}}}{K_X + \dfrac{X_S}{X_{BH}}} \right) \times \left(HetAirYes + \eta_h \times AirNo \times NO_3Yes \right) \times X_{BH}$
Hydrolysis of entrapped organic nitrogen	$k_H \times \left(\dfrac{\dfrac{X_S}{X_{BH}}}{K_X + \dfrac{X_S}{X_{BH}}} \right) \times \left(HetAirYes + \eta_h \times AirNo \times NO_3Yes \right) \times X_{BH} \times \dfrac{X_{ND}}{X_S}$
Ammonification of soluble organic nitrogen	$k_A \times S_{NH} \times X_{BH}$

Table 6 – MantisIW Volatilization Parameters

Symbol	Description	Units
Volatilization Rates		
$k_{V,OS}$	Volatilization rate for oxygenated solvents	1/d
$k_{V,HS}$	Volatilization rate for halogenated solvents	1/d
$k_{V,ALSC}$	Volatilization rate for short-chain aliphatic compounds	1/d
$k_{V,ARM}$	Volatilization rate for mono-cyclic aromatic compounds	1/d
$k_{V,PH}$	Volatilization rate for toxic or inhibitory compounds	1/d
$k_{V,ARH}$	Volatilization rate for halogenated aromatic compounds	1/d
Henry's Law Coefficients		
H_{OS}	Henry's Law coefficient for oxygenated solvents	m^3 liquid / m^3 gas
H_{HS}	Henry's Law coefficient for halogenated solvents	m^3 liquid / m^3 gas
H_{ALSC}	Henry's Law coefficient for short-chain aliphatic compounds	m^3 liquid / m^3 gas
H_{PH}	Henry's Law coefficient for toxic or inhibitory compounds	m^3 liquid / m^3 gas
H_{ARM}	Henry's Law coefficient for mono-cyclic aromatic compounds	m^3 liquid / m^3 gas
H_{ARH}	Henry's Law coefficient for halogenated aromatic compounds	m^3 liquid / m^3 gas

Table 7 – Definition of Switching Functions Used in MantisIW Model

Switching Function	Definition	Description
HetAirYes	$\left(\dfrac{S_O}{K_{OH} + S_O}\right)$	Used to limit aerobic heterotrophic growth at low dissolved oxygen concentrations.
NitAirYes	$\left(\dfrac{S_O}{K_{OA} + S_O}\right)$	Used to limit nitrifier growth at low dissolved oxygen concentrations.
AirNo	$\left(\dfrac{K_{OH}}{K_{OH} + S_O}\right)$	Used to limit anoxic heterotrophic growth at high dissolved oxygen concentrations.
AllowNitDenit	$\left(\dfrac{K_{AD}}{K_{AD} + S_O}\right)$	Used instead of *AirNo* if user wishes to allow for simultaneous nitrification/denitrification by adjusting the value of K_{AD}.
NH₃Yes	$\left(\dfrac{S_{NH}}{K_{NH} + S_{NH}}\right)$	Used to limit heterotrophic biomass growth at low ammonium concentrations.
PO₄Yes	$\left(\dfrac{S_P}{K_{PO} + S_P}\right)$	Used to limit biomass growth at low soluble ortho-phosphate concentrations.
NO₃Yes	$\left(\dfrac{S_{NO}}{K_{NO} + S_{NO}}\right)$	Used to limit anoxic heterotrophic growth at low nitrate concentrations.
AlkYes	$\left(\dfrac{S_{ALK}}{K_{ALK} + S_{ALK}}\right)$	Used to limit biomass growth at low alkalinity concentrations.

Table 8 – MantisIW Stoichiometric Coefficients

Symbol	Description	Units
Y_H	Yield for heterotrophic biomass	g cell COD/g COD utilized
$Y_{H,OS}$	Yield for heterotrophic biomass on oxygenated solvents	g cell COD/g COD utilized
$Y_{H,HS}$	Yield for heterotrophic biomass on halogenated solvents	g cell COD/g COD utilized
$Y_{H,ALSC}$	Yield for heterotrophic biomass on short-chain aliphatic compounds	g cell COD/g COD utilized
$Y_{H,ALLC}$	Yield for heterotrophic biomass on long-chain aliphatic compounds	g cell COD/g COD utilized
$Y_{H,ARM}$	Yield for heterotrophic biomass on mono-cyclic aromatic compounds	g cell COD/g COD utilized
$Y_{H,ARP}$	Yield for heterotrophic biomass on adsorbed poly-cyclic aromatic compounds	g cell COD/g COD utilized
$Y_{H,ARH}$	Yield for heterotrophic biomass on adsorbed halogenated aromatic compounds	g cell COD/g COD utilized
$Y_{H,PH}$	Yield for heterotrophic biomass on toxic or inhibitory compounds	g cell COD/g COD utilized
$Y_{H,COL}$	Yield for heterotrophic biomass on adsorbed colloidal material	g cell COD/g COD utilized
Y_A	Yield for nitrifying biomass	g cell COD/g N utilized
Y_{Sulfur}	Yield for sulfur oxidizing biomass	g cell COD/g S utilized
f_u	Fraction of biomass leading to particulate products	g COD/g cell COD
$ixbn$	Nitrogen fraction of active biomass	g N/g cell COD
$ixun$	Nitrogen fraction of endogenous/inert mass	g N/g COD
$ixbp$	Phosphorus fraction of active biomass	g P/g cell COD
$ixup$	Phosphorus fraction of endogenous/inert mass	g P/g COD

Table 9 – MantisIW Adsorption Parameters

Symbol	Description	Units
$K_{A,ALLC}$	Adsorption rate for long-chain aliphatic compounds	L/(mg COD·d)
$K_{A,ARP}$	Adsorption rate for poly-cyclic aromatic compounds	L/(mg COD·d)
$K_{A,ARH}$	Adsorption rate for halogenated aromatic compounds	L/(mg COD·d)
$K_{A,COL}$	Adsorption rate for colloidal material	L/(mg COD·d)
F_{max}	Fraction of adsorption sites available	Dimensionless

Table 10 – MantisIW Kinetic Parameters for Heterotrophic Growth (Part 1)

Symbol	Description	Units
Growth on Soluble Substrates		
μ_H	Maximum specific growth rate on readily biodegradable substrate	1/d
K_S	Half-saturation coefficient for readily biodegradable substrate	mg COD/L
$\mu_{H,OS}$	Maximum specific growth rate on oxygenated solvents	1/d
$K_{S,OS}$	Half-saturation coefficient for oxygenated solvents	mg COD/L
$\mu_{H,HS}$	Maximum specific growth rate on halogenated solvents	1/d
$K_{S,HS}$	Half-saturation coefficient for halogenated solvents	mg COD/L
$\mu_{H,ALSC}$	Maximum specific growth rate on short-chain aliphatic compounds	1/d
$K_{S,ALSC}$	Half-saturation coefficient for short-chain aliphatic compounds	mg COD/L
$\mu_{H,ARM}$	Maximum specific growth rate on mono-cyclic aromatic compounds	1/d
$K_{S,ARM}$	Half-saturation coefficient for mono-cyclic aromatic compounds	mg COD/L
$\mu_{H,PH}$	Maximum specific growth rate on toxic or inhibitory compounds	1/d
$K_{S,PH}$	Half-saturation coefficient for toxic or inhibitory compounds	mg COD/L
$K_{I,PH}$	Inhibition coefficient for toxic or inhibitory compounds	$(\text{mg COD/L})^2$
Growth on Adsorbed Substrates		
$\mu_{H,ALLC}$	Maximum specific growth rate on long-chain aliphatic compounds	1/d
$K_{S,ALLC}$	Half-saturation coefficient for long-chain aliphatic compounds	mg COD/L
$\mu_{H,ARP}$	Maximum specific growth rate on adsorbed poly-cyclic aromatic compounds	1/d
$K_{S,ARP}$	Half-saturation coefficient for adsorbed poly-cyclic aromatic compounds	mg COD/L
$\mu_{H,ARH}$	Maximum specific growth rate on adsorbed halogenated aromatic compounds	1/d
$K_{S,ARH}$	Half-saturation coefficient for adsorbed halogenated aromatic compounds	mg COD/L
$\mu_{H,COL}$	Maximum specific growth rate on adsorbed colloidal material	1/d
$K_{S,COL}$	Half-saturation coefficient for adsorbed colloidal material	mg COD/L
Anoxic Growth		
η_g	Anoxic growth reduction factor	Dimensionless
Decay		
b_H	Decay rate for heterotrophic organisms	1/d

Table 11 – MantisIW Kinetic Parameters for Heterotrophic Growth (Part 2)

Symbol	Description	Units
Hydrolysis		
k_H	Maximum specific hydrolysis rate	1/d
K_X	Half-saturation coefficient for hydrolysis	g COD / g cell COD
η_h	Anoxic hydrolysis reduction factor	Dimensionless
Ammonification		
k_A	Ammonification rate	L/(mg COD·d)
Switching Function Half-Saturation Coefficients		
K_{OH}	Oxygen half-saturation coefficient for heterotrophs	mg O_2/L
K_{NO}	Nitrate half-saturation coefficient	mg N/L
K_{NH}	Ammonia (as nutrient) half-saturation coefficient	mg N/L
K_{PO}	Phosphorus (as nutrient) half-saturation coefficient	mg P/L
K_{ALK}	Alkalinity half-saturation coefficient	mole/m^3
K_{AD}	Anoxic oxygen half-saturation coefficient for heterotrophs	mg O_2/L

Table 12 – MantisIW Kinetic Parameters for Nitrifiers and Sulfur Oxidizers

Symbol	Description	Units
Nitrifiers		
μ_A	Maximum specific growth rate for nitrifiers	1/d
K_{NA}	Ammonia half-saturation coefficient for nitrifiers	mg N/L
K_{OA}	Oxygen half-saturation coefficient for nitrifiers	mg N/L
b_A	Decay rate for nitrifiers	1/d
Sulfur Oxidizers		
$\mu_{A,Sulfur}$	Maximum specific growth rate for sulfur oxidizers	1/d
$K_{A,Sulfur}$	Sulfur half-saturation coefficient	mg N/L
$b_{A,Sulfur}$	Decay rate for sulfur oxidizers	1/d

RESULTS

Preliminary Testing of the Industrial Activated Sludge Model

The industrial activated sludge model was implemented in the GPS-X™ wastewater treatment plant simulator, which includes models for other required processes such as clarification and flow routing. The industrial activated sludge model was tested using data from an activated sludge process treating pulp and paper wastewater. The plant treats an average of 3.3 Mgal/d and includes primary clarification, step-feed activated sludge, and final clarification in two parallel trains. Activated sludge is wasted from the aerobic reactors. A model of the secondary treatment system was developed in GPS-X™ and is shown in Figure 3.

Influent data were available in the form of daily flow rates, 5-day biochemical oxygen demand (BOD_5), COD, total suspended solids (TSS), and volatile suspended solids (VSS). Detailed information concerning the compounds present in the influent was not available. It was assumed that the influent solids were mainly comprised of insoluble fibers. The remaining soluble material was thought to be primarily organic compounds such methanol and formic acid. The influent also contains a significant amount of reduced sulfur compounds (~ 25 mg/L). The primary effluent COD was categorized as follows:

- Total COD (average of 530 mg/L)
    - 80% soluble COD
    - 20% particulate
- Soluble COD
    - 90% oxygenated solvents
    - 10% inert COD
- Particulate COD
    - 99% inert COD
    - 1% slowly biodegradable COD

A VSS/TSS ratio of 0.6 was used. The default MantisIW kinetic and parameter values were used.

The plant was simulated for a period of 30 days using historical operating data. The simulated and measured results for the mixed liquor suspended solids (MLSS) and mixed liquor volatile suspended solids (MLVSS) are given in Figure 4. Similarly, the simulated and measured results for the effluent volatile suspended solids (VSS) and effluent BOD are shown in Figure 5. As shown, the model is able to predict the plant data reasonably well in most cases considering the variability typically associated with wastewater measurements. Given the aeration system configuration used in the plant, the model predicted dissolved oxygen (DO) concentrations in the reactor that were within the ranges of the periodic DO measurements taken at the plant. The model predicted that the reduced sulfur compounds would be entirely oxidized to sulfates.

Testing of the model is ongoing. Currently, the model parameters are being fine-tuned using historical data from industrial ASP's.

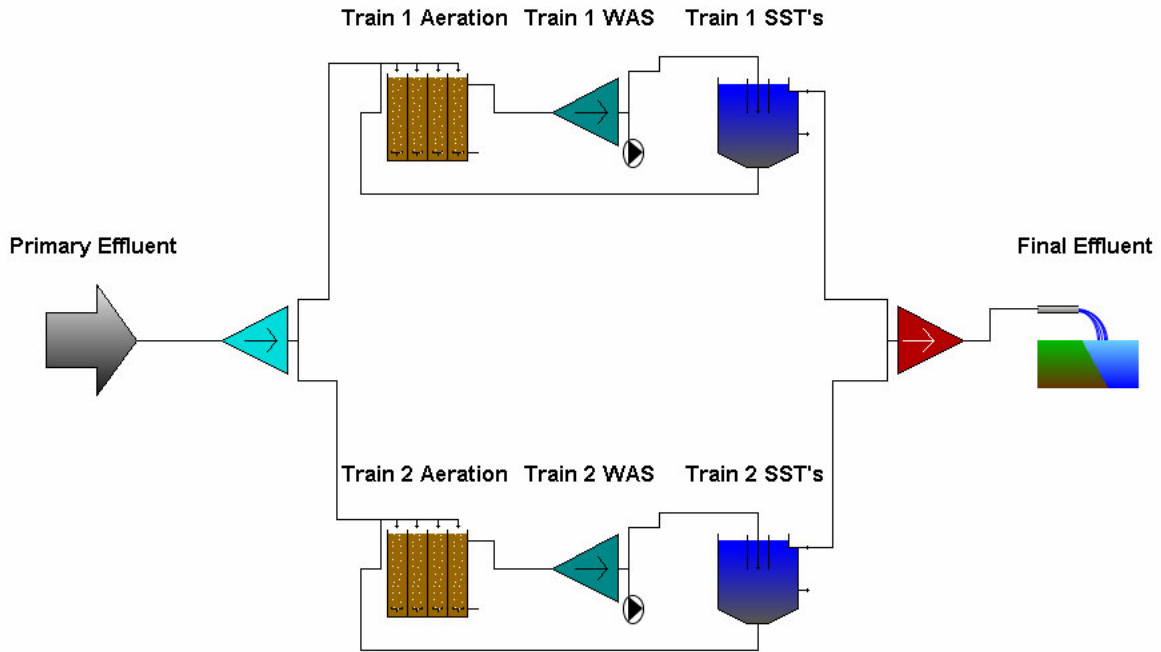**Figure 3 – Plant Model as Represented in GPS-X™**

Figure 4 – Predicted and Measured MLSS and MLVSS in One Train of Activated Sludge Process
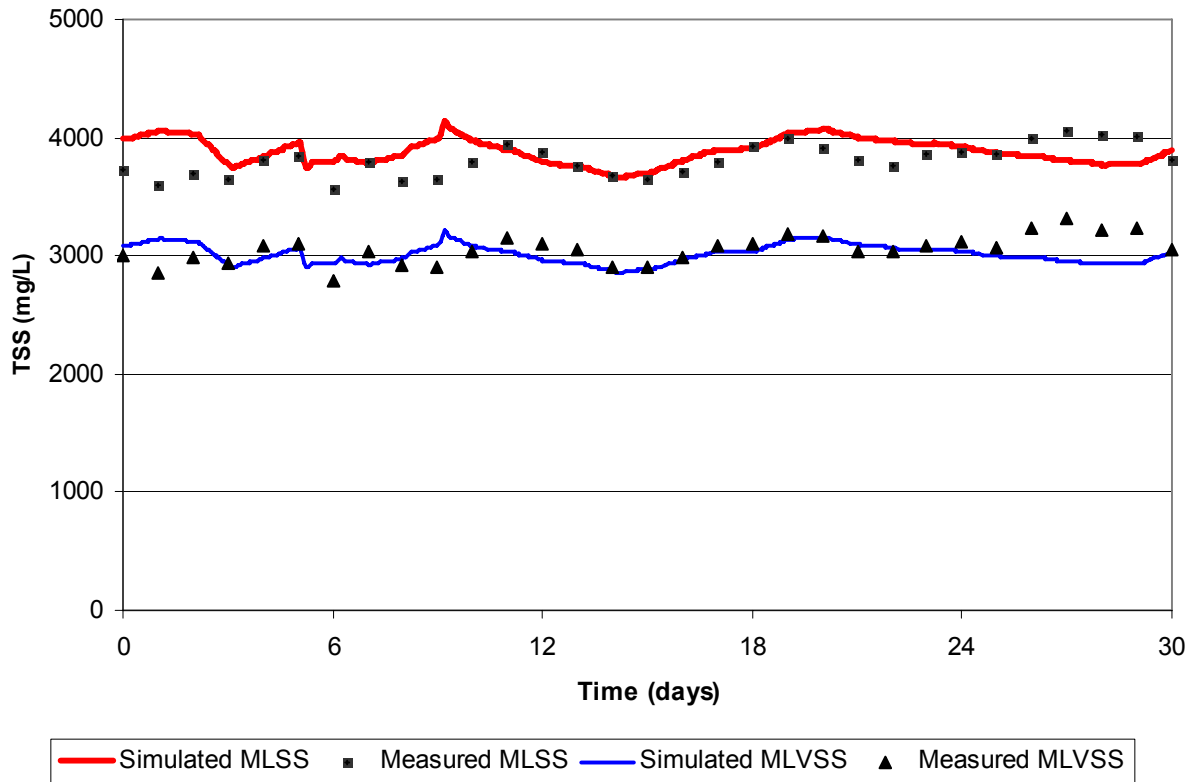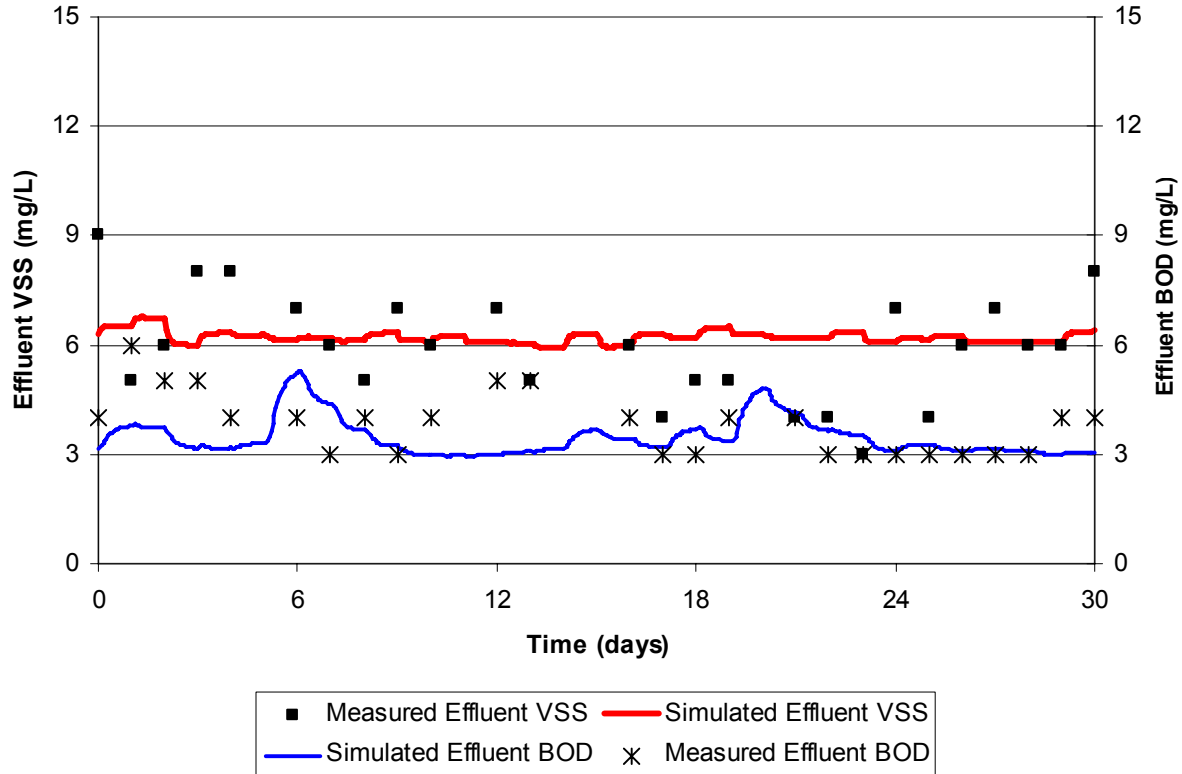
Figure 5 – Predicted and Measured Effluent BOD and VSS

DISCUSSION

The industrial activated sludge model, MantisIW, provides a general framework for the modeling of industrial activated sludge treatment processes. It provides sufficient detail in terms of the wastewater characterization and the biological and physical processes modeled to allow for application of the model in a wide variety of industries. The user has flexibility in choosing which aspects of the model to apply in a given situation by using the appropriate influent categorization and the available model components. The inclusion of multiple new model components allows for tracking of a variety of industrial pollutants.

The new features of the model include the following:

- *New classification of organic influent COD*
- *Multiple transformation processes for new COD components*: volatilization, adsorption, and biological growth. Certain COD components can undergo volatilization and biological oxidation simultaneously.
- *Improved description of volatilization*: current activated sludge models do not separately account for contributions from surface volatilization and air stripping due to aeration.
- *Impact of nutrient and alkalinity requirements on all biological growth processes in model*: all processes can be limited if nutrient or alkalinity concentrations are low. The impact of sulfur oxidation on alkalinity is included.

The model also includes the following features:

- Simultaneous nitrification/denitrification
- Inhibited biological oxidation of toxic compounds such as phenols
- Biological oxidation of reduced sulfur compounds
- Modeling the fate of colloidal material

While this newly developed model is a significant step forward in the modeling of industrial activated sludge treatment plants, the model will continue to be upgraded and developed in the future. Future improvements will include:

- Development of an influent characterization tool that will allow the user to directly define the influent characteristics in terms of chemical compounds instead of COD.
- Application of the model to other industrial biological treatment processes such as moving bed bioreactors (MBBRs) and membrane bioreactors (MBRs).
- Modeling the impact of toxic inhibition on all biological growth processes.
- Modeling of volatilization due to mechanical aeration.

The MantisIW model will provide significant advantages over existing activated sludge models for domestic wastewater. Potential uses for the model include:

- Design: comparing and testing of alternatives
- Research: experimental design
- Plant Operations: trouble-shoot plant problems, improve control strategies, design plant monitoring programs, decide on placement of online instruments
- Training: training of plant staff

CONCLUSIONS

A new activated sludge model has been developed that provides a general framework for the modeling of industrial activated sludge treatment processes. The model combines the ASM1 biological model with a new categorization of the influent COD and added biological and physical transformations. The model stoichiometry and process rate equations have been provided. The parameter values are taken from the literature and other sources such as the TOXCHEM+™ (Hydromantis, 2006b) predictive fate modeling package. Preliminary testing of the model has been done using data from an activated sludge plant treating pulp and paper wastewater. Testing of the model is ongoing. Currently, the model parameters are being fine-tuned using historical data from industrial ASP's. Future work will include development of an influent characterization tool, modeling the impact of toxic inhibition on all biological growth processes, and modeling of the volatilization due to mechanical aeration.

REFERENCES

Baker, A.J. (1994) Modeling Activated Sludge Treatment of Petroleum and Petrochemical Wastes. PhD. Thesis, McMaster University, Hamilton, Ontario, Canada.

Bury, S.J.; Groot, C.K.; Huth, C.; Hardt, N. (2002) Dynamic simulation of chemical industry wastewater treatment plants. *Wat. Sci. Technol.*, **45** (4-5), 355.

Gaudy, A.F., Jr.; Gaudy, E.T. (1980) Microbiology for Environmental Scientists and Engineers. McGraw-Hill, NY.

Goodfellow, J., Malyk, B., Hahn, D., Johnson, D. (2004) Evaluation of Biological Phosphorous Removal Versus Chemical Phosphorous Removal at a Potato Processing Facility. *Proceedings of the WEF/A&WMA 10th Annual Industrial Wastes Technical and Regulatory Conference*, August 22-25, Philadelphia, Pennsylvania.

Henze, M.; Gujer, W.; Mino, T.; van Loossdrecht, M. (2000) *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*; Scientific and Technical Report No 9; IWA Publishing, London, England.

Hydromantis, Inc. (2006a) GPS-X 5.0 Technical Reference Manual. Hamilton, ON, Canada.

Hydromantis, Inc. (2006b) TOXCHEM+ V3.35 Predictive Fate Software. Hamilton, ON, Canada.

Matter-Muller, C.W.; Gujer, W.; Giger, W. (1981) Transfer of Volatile Substances from Water to the Atmosphere. *Water Research*, **15**, 1271.

Schraa, O.; Belia, E.; Churn, C.C. (2004) The Use of Process Modeling to Investigate the Performance of a Large Industrial Wastewater Treatment Plant. *Proceedings of the Water Environment Federation's 77th Annual Technical Exhibition and Conference*, October 2-6, New Orleans, Louisiana.

Snowling, S.D.; Malyk, W.J. (2002) Using Dynamic Simulation as a Decision-Making Tool, A Successful Industrial Wastewater Application. *Proceedings of the 8th Annual WEF Industrial Wastes Technical and Regulatory Conference*, Atlantic City, NJ, Aug. 11-14, 2002.

Stricker, A.E.; Racault, Y. (2005) Application of Activated Sludge Model No. 1 to biological treatment of pure winery effluents: case studies. *Wat. Sci. Technol*, **51** (1), 121.

Takács, I.; Lockwood, S.; Caplis, J.R. (1998) Simulation model helps manufacturing facility maintain regulatory compliance, optimize treatment processes, and train operators. *Industrial Wastewater*, May/June 1998.